Damage Modeling of Graded Ti-based Composites Using Repeated Unit Cell Approach

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***Abstract*-In the present study, macroscopic mechanical behaviors of titanium-based functionally graded biomaterials (FGMs) under the influence of composite damage have been investigated using the repeated unit cell approach. Based on the proposed method, the FGMs were idealized to be composed of finite uniform layers, each of which is represented by one repeated unit cell. The titanium (Ti) matrix is modeled as an isotropic hardening elastic plastic solid following the incremental (J_2) theory of plasticity. As the strength and fracture toughness of hydroxyappatite (HA) inclusion is very weak as compared with the Ti metal, the HA particles may be broken firstly when the composite is subjected to an excessive load. The brittle failure criterion has been implemented in the VUMAT subroutine using the finite element software ABAQUS. A uniaxial tension test along the *y*-axis of the unit cell has been simulated. The simulation results show that the load-bearing capability of Ti/HA FGMs will decrease rapidly with the increase in the volume fraction of HA. Due to the absence of the load bearing capability of HA, the mechanical behaviors of unit cell are similar to those of a porous structure and the applied load is entirely carried by the Ti matrix. The computational results indicate that this method is capable of predicting the failure process of Ti/HA FGMs.**

Keywords- Functionally Graded Biomaterials; Repeated Unit Cell; Brittle Failure; Damage

I. INTRODUCTION

In recent years, there has been increasing attention to the development of biocomposites for load-bearing orthopedic applications, because the mechanical and biological properties of biocomposites can be tailored for specific application by varying the amount and type of constituent materials [1-5]. Hydroxyapatite (HA), a bioactive ceramic material, has outstanding osteoconductivity, enabling bone to form or to adhere to its surface [6, 7]. However, the low tensile strength and poor impact strength of HA have hindered its use in load-bearing applications. Titanium (Ti) and its alloys have been used in several implant applications due to its excellent mechanical behaviors and bioinert oxide surface. However, they suffer certain disadvantages, such as poor osteoinductive properties. Therefore, significant research efforts have been made on improving bioactivity of Ti by coating its oxide surface with HA [8]. However, the HA coating layer often breaks down mechanically. To resolve the limitation of the HA coating, the conception of functionally graded biomaterials (FGMs) may be applied for designing implant. Titanium/Hydroxyapatite (Ti/HA) FGMs can be fabricated successfully by a laser rapid forming method [9], which makes full use of the excellent bioactivity of HA as well as the high strength and toughness of Ti. This type of implant can provide more Ti for the upper part to withstand the occlusal force, and more apatite for the lower part for implantation into the jaw bone [10].

Material damage and its evolution govern the fracture behavior of FGMs that provides essential knowledge for damage tolerance and defect assessment in structural design. In contrast with the relatively extensive literature on the quasi-static and dynamic behavior of cracks in FGMs [11-13], attempts to study the material damage of FGMs quantitatively by relating the micro-structural damage to the mechanical response of a FGM have not been reported. It is usually very difficult and almost impossible to investigate FGM structural problems analytically. Therefore, applications of finite element method (FEM) [14] in investigating fracture behaviors of FGMs under mechanical or thermal loading have been an active area recently. Under excessive loading, the brittle failure of HA particles can occur in Ti/HA FGMs. So far, there is no method with which internal damage phenomena and the microscopic fracture process of FGMs can be satisfactorily predicted. Therefore, it is necessary to establish a method of bridging the microstructural damage mechanical mechanism and the macrostructural behaviour.

This study, based on the previous work on investigating the microscopic mechanical behavior of Ti/HA FGMs [15], not only provided the detailed implementation of the previous work but also focused on modeling the effect of composite damage on the macroscopic mechanical behavior of Ti/HA FGMs. In order to consider two phase microstructure and gradual variation of mechanical properties in FGMs, a repeated unit cell approach has been proposed. And the brittle failure criteria of HA has been implemented in the VUMAT subroutine using the finite element software package—ABAQUS. Using the proposed method, the microscopic damage behavior of Ti/HA composite and hence the macroscopic mechanical behavior of Ti/HA FGMs could be simulated.

II. REPEATED UNIT CELL APPROACH

Due to graded microstructure, the local field in FGMs not only changes greatly between two phases, but also

varies spatially in the gradation direction. The distribution of HA particles has a graded variation in the longitudinal direction. For simplicity, the shape of HA particles was idealized as spherical. As shown in Fig. 1, the FGM was idealized to be composed of finite uniform layers and each layer was represented by one repeated unit cell. In this paper, the FGM was divided into five layers, in which HA particles were spherical and the volume fractions of HA are 0%, 10%, 20%, 30% and 40%, respectively. By varying the volume fractions of HA, these five layers were expressed as HA0-Ti, HA10-Ti, HA20-Ti, HA30-Ti and HA40-Ti. For example, HA10-Ti was designated as 10% of HA in the composite by volume. Moreover, the particle distribution was approximated by arranging the particles in a face-centered cubic (FCC) packing. With this packing pattern, particle volume fraction in this model could reach 74%. Due to symmetry, only one-eighth of the FCC packing is needed for analysis.

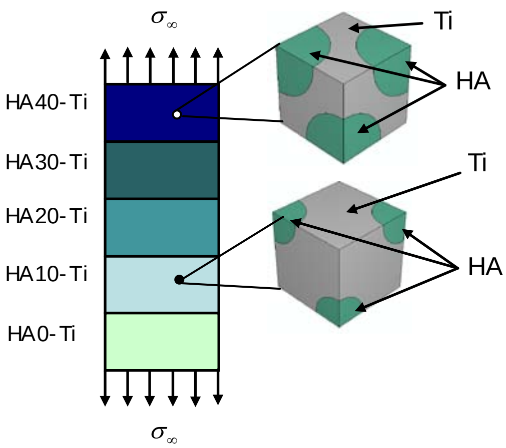


Fig. 1 Schematic illustration of two-phase functionally graded particulate material

To investigate the effect of filler particle volume fraction on the mechanical properties of FGMs, five representative unit cells were established in this paper. The required filler radius can be determined from

$$r = \left(\frac{3L^3\phi}{2\pi}\right)^{1/3}$$

where ϕ is the volume fraction of HA, and L is the length of the cubic unit cell. Periodic boundary conditions were used to force the particle and matrix to remain in its original shape. The cell was loaded in tension along the y-direction. The cell was forced to maintain its regular cubic shape after deformation due to the effect of the surrounding material and the loading character [16].

III. CONSTITUTIVE EQUATIONS OF TI AND HA

The Ti matrix was modeled as an isotropic hardening elastic plastic solid following the incremental (J2) theory of plasticity. And the corresponding constitutive relation is available in FEM software—ABAQUS. The strength and fracture toughness of HA particles are very weak as compared with the Ti metal. The HA particles may be broken firstly when the composite is subjected to an excessive load. According to the experimental results, the deformation behavior of the HA particle can be characterized by a purely elastic constitutive law. The generalized Hooke's law is satisfactory to reflect the deformation behavior of the HA particle in the biocomposite [17]. The constitutive equation and the failure criterion of HA can be expressed as follows:

$$\left.\begin{array}{ll} \sigma = D\varepsilon, & \sigma_M < \sigma_b \\ \sigma = 0, & \sigma_M \geq \sigma_b \end{array}\right\}$$

where σ, ε, and D are the stress tensor, the strain tensor and the elastic constitutive matrix, respectively. Moreover, σ_M is the von Mises stress, and σ_b represents the ultimate strength, and D can be defined as:

$$D = \frac{E}{2(1+\nu)(1-2\nu)}\begin{bmatrix} 2(1-\nu) & 2\nu & 2\nu & 0 & 0 & 0 \\ 2\nu & 2(1-\nu) & 2\nu & 0 & 0 & 0 \\ 2\nu & 2\nu & 2(1-\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-2\nu \end{bmatrix}$$

where E and ν are Young's modulus and Poisson ratio, respectively.

The constitutive equation and brittle failure criterion of HA have been implemented in the VUMAT subroutine of ABAQUS/Explicit. If material points satisfied the failure criterion, they would be set to zero stress and strain and eliminated from the model. Once a material point has been flagged as a "deleted" status, it could not be reactivated. The corresponding material parameters of Ti and HA are summarized in Table 1.

TABLE 1 MATERIAL PROPERTIES OF TI [12] AND HA [13]

Material	E **(GPa)**	ν	σ_s **(MPa)**	σ_b **(MPa)**	ρ **(kg/m³)**
Ti	110	0.35	450	800	4500
HA	40	0.27	--	100	3219

IV. COMPUTATIONAL RESULTS AND DISCUSSION

In this section, uniaxial tension tests along the y-axis of the repeated unit cells have been simulated using the proposed method and user-defined material subroutine. The macroscopic stress-strain curves are obtained and illustrated in Fig. 2. In this figure, when the von Mises stress of the HA particle reaches a value of 100 MPa, the particle failed and lost the load-bearing capability. The load decreases abruptly due to the presence of the brittle failure of the HA particles. And the strain softening phenomenon can be observed in the unit cell. Figure 2 also shows that the volume fraction of HA affects the mechanical behaviors of Ti/HA FGMs evidently. It is noted that the load-bearing capability of the composite decreases rapidly with the increase in the volume fraction of HA. According to the rule of mixture based on Reuss equal stress assumption, the apparent stress strain relation of graded structure was derived and plotted in Fig. 3.

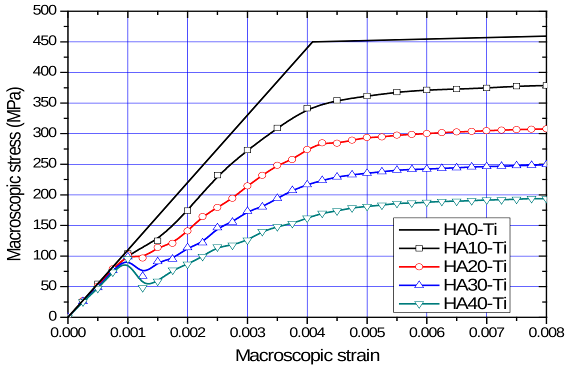


Fig.2 Macroscopic stress-strain relations predicted by the repeated unit cell model

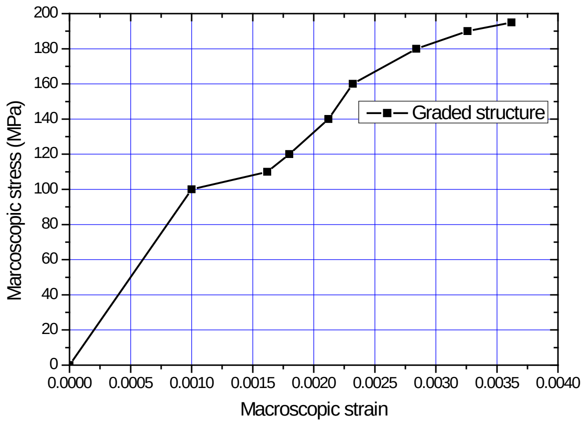
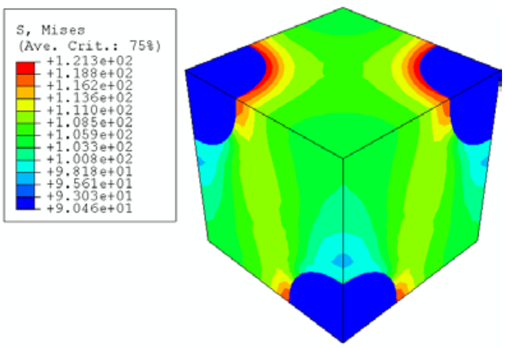


Fig.3 The apparent stress-strain relation of the graded structure

Figure 4(a) illustrates the von Mises stress contour of HA10-Ti composite before the failure of HA occurs. It can be seen that the von Mises stress distribution is interrupted at the interface between Ti and HA. Because of the higher Young's modulus in the Ti matrix, the stress of HA particle is much larger than that of the Ti matrix. Due to the absence of the load bearing capability of HA, the mechanical behaviors of the composite are similar to those of a porous one, and the applied load is entirely carried by the Ti matrix as shown in Fig. 4(b). Moreover, the work hardening of Ti matrix would continue with the increase in the strain of the unit cell. Bone, a kind of functionally graded material structure, can be modelled by the proposed method to determine its macroscopic mechanical response and the local damage in its structure.



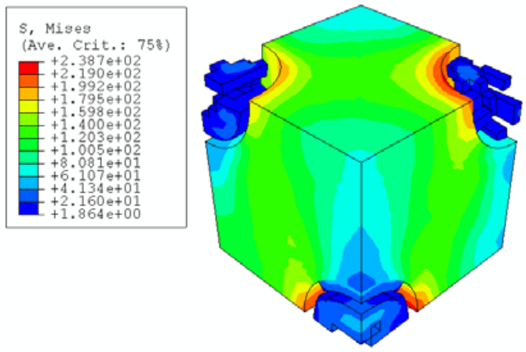


Fig.4 Von Mises stress contour of unit cell (a) no damage, (b) particle fracture

V. CONCLUSIONS

In this paper, a repeated unit cell approach with consideration of the two phase microstructure and gradual variation of FGMs has been developed. And the brittle failure criteria of HA has been implemented in the Vumat subroutine using the finite element software—ABAQUS. Using the proposed method, the macroscopic and microscopic mechanical behaviors of Ti/HA FGMs have been investigated, and the effect of the failure of HA on the Ti/HA FGMs has also been incorporated in modeling. The computational results indicate that this method can be used for simulating the microscopic damage behavior of Ti/HA composite and hence predicting the macroscopic mechanical response of Ti/HA FGMs.

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